Solvability of Some Statistical Mechanical Systems

A. J. Guttmann[1] and I. G. Enting[2]
[1]*Department of Mathematics, The University of Melbourne Parkville, Victoria 3052, Australia*
[2]*Commonwealth Scientific and Industrial Research Organization, Division of Atmospheric Research, Private Bag No. 1, Mordialloc, Victoria 3195, Australia*
(Received 26 September 1995)

We describe a numerical procedure that clearly indicates whether or not a given statistical mechanical system is solvable (in the sense of being expressible in terms of D-finite functions). If the system is not solvable in this sense, any solution that exists must be expressible in terms of functions that possess a natural boundary. We provide compelling evidence that the susceptibility of the two-dimensional Ising model, the generating function of square lattice self-avoiding walks and polygons and of hexagonal lattice polygons, and directed animals are in the "unsolvable" class.

PACS numbers: 05.20.–y, 02.60.–x, 05.50.+q

Some of the most famous results in mathematics involve a proof of the intrinsic unsolvability of certain problems—such as the determination of the roots of polynomial equations of a degree greater than 4. In theoretical physics such results are largely unknown. In this Letter we take a first step towards filling this gap by providing a powerful numerical technique that provides strong evidence for the unsolvability of certain prominent problems in equilibrium statistical mechanics in terms of the "standard" functions of mathematical physics. While falling short of a proof, the method is of widespread applicability.

There is a short but celebrated list of models in statistical mechanics for which closed form solutions are available. These include the zero-field partition function [1] and spontaneous magnetization [2] of the two-dimensional Ising model, the square lattice dimer model [3,4], the six-vertex model [5], the eight-vertex model [6], and the hard hexagon model [7].

There are other models which are perhaps more obviously viewed as combinatorial problems, rather than as models in statistical mechanics, for which the exact solution is also known. These include a range of polygon enumeration problems by both perimeter and area, such as staircase polygons, convex polygons, and row-convex polygons [8,9], also walk models, such as the partially directed self-avoiding walk [10], the solid-on-solid model with field and surface interactions [11], and lattice animal models such as the enumeration of directed column-convex animals [12] and directed animals on the square and triangular lattices [13].

There is an even longer list of celebrated unsolved problems, prominent among which are the susceptibility of the two-dimensional Ising model [14], the partition function of the two-dimensional Ising model in a field, the three-dimensional Ising model, the two-dimensional self-avoiding walk and polygon model, two-dimensional percolation, two-dimensional directed percolation [15], and directed animals on the hexagonal lattice [16] to name but a few.

The first question we wish to address in studying this latter class is what is meant by a solution. Restricting consideration to functions of a single variable, such as temperature or perimeter, one ideally desires a simple closed form expression, such as that obtained [2] for the Ising model spontaneous magnetization. Less restrictively, one may seek a differential or difference equation which can be solved to yield the analytic structure. A more restrictive class is formed by the *D-finite* functions [17], defined as those functions which are solutions of a linear ordinary differential equation of finite order with polynomial coefficients. This class contains most of the solved models mentioned above. Certainly the zero-field partition function and magnetization of the Ising model fall into this class. However, we provide compelling evidence below that the susceptibility does not.

We first consider the zero-field reduced partition function for the *anisotropic* model, defined by $\Lambda \times (t_1, t_2) = \lim_{V\to\infty}[Z(K_1, K_2)/2\cosh K_1 \cosh K_2]^{1/V}$, where $t_i = \tanh K_i$ and V is the number of lattice sites. Writing

$$\ln\Lambda(t_1, t_2) = \sum_{n,m} a_{n,m} t_1^{2m} t_2^{2n} = \sum_n R_n(t_1^2) t_2^{2n} ,$$

Baxter [18] has shown that

$$R_n(t_1^2) = P_{2n-1}(t_1^2)/(1 - t_1^2)^{2n-1}.$$

That is to say, the functions R_n are rational, with numerators and denominators of degree $2n - 1$, and with the denominator having a particularly simple structure. In the complex t_1^2 plane, there is a singularity only at $t_1^2 = 1$.

In fact [18], due to the existence of the inversion relation

$$\ln\Lambda(t_1, t_2) + \ln\Lambda(1/t_1, -t_2) = \ln(1 - t_1^2),$$

and the obvious symmetry relation $\Lambda(t_1, t_2) = \Lambda(t_2, t_1)$, the form of the denominator is sufficient to determine, order by order, the numerator polynomials P_n. That is to say, the complete Onsager solution is implicitly determined by these two functional equations and the fact that the only singularity of the denominator occurs at

 0031-9007/96/76(3)/344(4)$06.00

$t_1^2 = 1$. It was this realization that prompted a corresponding study [19] of the susceptibility.

The zero-field susceptibility of the triangular lattice Ising model, with coupling constants K_1, K_2, K_3, and $t_i = \tanh(K_i)$, satisfies [20] an inversion relation $\chi(t_1, t_2, t_3) + \chi(-t_1, -t_2, 1/t_3) = 0$. Since the anisotropic square lattice can be obtained by setting one of the anisotropic coupling constants to zero, it follows that the anisotropic square lattice susceptibility satisfies the inversion relation $\chi(t_1, t_2) + \chi(1/t_1, -t_2) = 0$, as well as the symmetry relation $\chi(t_1, t_2) = \chi(t_2, t_1)$. We may write the susceptibility as

$$\chi(t_1, t_2) = \sum_{m,n=0}^{\infty} c_{m,n} t_1^m t_2^n = \sum_{n=0}^{\infty} H_n(t_1) t_2^n.$$

The first three values $H_n(x), n = 1, 2, 3$, were given in [21], $H_5(x)$ (but not H_4) was given in [19], and we [22] recently reported the calculation of $H_n(x)$ for $n \leq 14$ by the finite-lattice method [23]. The first few values are

$$H_0(t) = \frac{1 + t}{1 - t},$$

$$H_1(t) = \frac{2(1 + t)^2}{(1 - t)^2},$$

$$H_2(t) = \frac{2(1 + 6t + 8t^2 + 6t^3 + t^4)}{(1 - t)^3(1 + t)},$$

$$H_3(t) = \frac{2(1 + 8t + 10t^2 + 8t^3 + t^4)}{(1 - t)^4},$$

$$H_4(t) = \frac{2(1 + t^{10} + 15(t + t^9) + 71(t^2 + t^8) + 192(t^3 + t^7) + 326(t^4 + t^6) + 388t^5)}{(1 - t^3)(1 - t)^4(1 + t)^3},$$

$$H_5(t) = \frac{2(1 + 16(t + t^7) + 64(t^2 + t^6) + 144(t^3 + t^5) + 166t^4 + t^8)}{(1 - t)^6(1 + t)^2},$$

$$H_6(t) = [2(1 + t^{18} + 25(t + t^{17}) + 220(t^2 + t^{16}) + 1149(t^3 + t^{15}) + 4081(t^4 + t^{14}) + 10768(t^5 + t^{13}) + 22083(t^6 + t^{12}) + 36283(t^7 + t^{11}) + 48543(t^8 + t^{10}) + 53446t^9)]/[(1 - t^3)^3(1 - t)^4(1 + t)^5].$$

In all cases enumerated, the numerator polynomial is unimodal and symmetric with positive coefficients. The denominator polynomial clearly has zeros at $t = 1$ for all n, as well as at $t = -1$ for $n = 2$ and $n \geq 4$. Our results show that for $n = 4$ and $n \geq 6$ (at least up to $n = 14$) there are zeros at $t^3 = 1$, and at $n = 12$ the first occurrence of zeros at $t^5 = 1$ appears. The numerator and denominator polynomials (with no common factors) are of equal degree, notably $1, 2, 4, 4, 10, 8, 18, 20, 26, 28, 34, 36, 48, 44, 62$ for $n = 0, 1, 2, \cdots, 14$, respectively. The rate of increase of degree with n is such that even if we knew the form of the denominator, the inversion relation and symmetry relation would be insufficient to implicitly yield the solution, unlike the case of the free energy. This is because the symmetry property gives the value of n coefficients from the previous H_n's, while the inversion relation means that only half the coefficients are needed. Together, this means that $2n$ coefficients of the numerator can be identified. This is precisely the number of numerator coefficients in the case of the free energy, but it is clear that the degree of the numerator polynomial in the case of the susceptibility is increasing faster than $2n$.

Nevertheless, we can obtain important information about the analytic structure of the solution. From [14], in which the susceptibility of the Ising model is expressed as an expansion in terms of $2k + 1$ particle excitations, the structure of the denominator of the H_n functions is clear. The lowest order terms of the series expansion are obtained from the 1-particle contribution. The 3-particle contribution starts at $O(t^8)$—corresponding to the first occurrence of the factor $(1 - t^3)$ in the denominator of $H_4(t)$, while the 5-particle contribution starts at $O(t^{24})$—corresponding to the first occurrence of the factor $1 - t^5$ in the denominator of $H_{12}(t)$. Now the susceptibility expansion in terms of $2k + 1$ particle excitations is a sum of infinite series, each series contributing only at steadily increasing powers of the high-temperature expansion variable t. As we have seen above, the contribution of the terms from the $2k + 1$ particle excitations, which first contribute at, say, $O(t^{2m})$, correspond to poles at $t^{2k+1} = 1$ in $H_m(t)$ in the anisotropic expansion above. Hence we can identify the first occurrence of the factor $1 - t^{2k+1}$ in the denominator with the first occurrence of a $2k + 1$ particle excitation.

From this observation, we see that the structure of $H_n(t)$ is that of a rational function whose poles all lie on the unit circle in the complex t plane, *such that poles become dense on the unit circle as n gets large.* This behavior implies (unless miraculous cancellation of almost all poles occurs at high order) that the functions $H_n(t)$, and hence $\chi(t_1, t_2)$ as a function of t_1 for t_2 fixed, (a) has a natural boundary, (b) is not algebraic, and (c), more loosely, cannot be expressed in terms of the "usual" functions of mathematical physics, such as elliptic integrals or solutions of the hypergeometric equation in general. More precisely, no D-finite function is a candidate. One family of functions that does suggest itself as a possible candidate is the q generalization of the standard functions of mathematical physics, which we have seen in a number of solutions already [7,11]. The q functions date back to Euler and Gauss, blossomed with the work of Ramanujan, and in recent years have migrated from number theory to the forefront of statistical mechanics [24,25].

This observed behavior suggests a new and powerful tool to investigate the analytic structure of a wide variety of problems. By generalizing to the anisotropic model, and studying the distribution of zeros of the denominators in the $H_n(t)$ functions and their analogs, we can distinguish between those that appear to be solvable in terms of standard functions—when there is just a finite number of singularities on the unit circle (usually just one)—and those which are not, with an infinite number of such singularities (signified numerically of course by a growing number of singularities as the number of H_n functions calculated grows). The partition function and susceptibility of the two-dimensional zero-field Ising model are paradigms, respectively, of each class, as we have just shown.

We have applied this approach to a number of other unsolved problems in statistical mechanics of two-dimensional systems, notably self-avoiding polygons on the square and hexagonal lattices. In both cases we can write the polygon generating function as

$$P(x,y) = \sum_{n=1}^{\infty} R_n(x^2) y^{2n}.$$

For square lattice polygons we find that R_n is a rational function of x^2, with numerator and denominator of equal degree. The denominator is $(1 - x^2)^{2n-1}$ for $n \leq 4$, but for $n > 4$ powers of $1 - x^4$ enter, and for $n > 6$ we see powers of $1 - x^6$ entering, while $n = 8$ marks the first occurrence of powers of $1 - x^8$.

For hexagonal lattice polygons (on a brickwork lattice, so that there are only two types of bond, horizontal and vertical) a similar pattern is observed, except that the numerator and denominator of the rational functions $R_n(x^2)$ are not of equal degree. The denominators always have zeros only on the unit circle in the complex x^2 plane, just at $x^2 = 1$ for $n \leq 3$, with powers of $1 - x^4$ appearing in the denominator at $n = 4$, powers of $1 - x^6$ entering at $n = 7$ and so on.

Thus we see the same pattern as in the Ising susceptibility, with the zeros of the denominator becoming dense on the unit circle. (Of course, we have not *proved* that this occurs, but the evidence is most persuasive). As before, this implies that the solution is not algebraic, and not D finite.

A similar situation has been noted for square lattice anisotropic self-avoiding walks [26]. That is, a buildup of zeros of the denominator of the $H_n(t)$ functions on the unit circle in the complex t plane. This implies that this function also fails to be D finite. This statement appears also to be true for hexagonal lattice directed animals [10,26]. Earlier work [19] on the three-dimensional anisotropic zero-field Ising model gives a strong hint that this model too is not D finite, though longer series are needed to be unequivocal. Full details of all the above calculations will be given elsewhere.

Finally, we note that a number of solvable problems, including staircase, convex, and row convex polygons, as well as the triangular lattice Ising model susceptibility along the disorder line, can be studied similarly. We first generalize to the anisotropic model and look at the structure of the H_n functions in the two-variable series. All are found to have a pole at only one point in the complex t plane (or its analog), consistent with our observation that this is a hallmark of a readily solvable model. The method is also applicable to three-dimensional systems, and to nontranslationally invariant problems such as directed animals (referred to above) and directed percolation [27].

Thus we believe that we have introduced a new and powerful numerical tool in the study of lattice statistical models. It allows one to clearly distinguish between models that are D finite—and hence likely to be readily solvable— and those that are not only not D finite, but display a natural boundary on the unit circle. The solution of this latter class will require more subtle mathematical approaches, the most obvious candidate for which are q generalizations of the standard functions.

We have benefited from discussions on this topic with many people. Notable among them are Rodney Baxter, Richard Brak, Omar Foda, Jean-Marie Maillard, Barry McCoy, Aleks Owczarek, Robert Shrock, Alan Sokal, Colin Thompson, and Dominic Welsh. We are particularly indebted to Andrew Conway and Iwan Jensen, who communicated their preliminary results on anisotropic self-avoiding walks, hexagonal lattice directed animals, and anisotropic directed percolation, and to Mireille Bousquet-Mélou, David Gaunt, Aleks Owczarek, and Alan Sokal for helpful comments on the manuscript.

[1] L. Onsager, Phys. Rev. **65**, 117 (1944).
[2] C. N. Yang, Phys. Rev. **85**, 808 (1952).
[3] P. W. Kasteleyn, Physica (Utrecht) **27**, 1209 (1961).
[4] H. N. V. Temperley and M. E. Fisher, Philos. Mag. **6**, 1061 (1961).
[5] E. H. Lieb, Phys. Rev. Lett. **18**, 1046 (1967); **19**, 108 (1967).
[6] R. J. Baxter, Phys. Rev. Lett. **26**, 832 (1971).
[7] R. J. Baxter, J. Phys. A **13**, L61 (1980).
[8] M. P. Delest, J. Math. Chem. **8**, 3 (1991).
[9] A. J. Guttmann, *Computer-Aided Statistical Physics*, AIP Conf. Proc. No. 248 (AIP, New York, 1992), p. 12.
[10] R. J. Brak, A. J. Guttmann, and S. G. Whittington, J. Phys. A **25**, 2437 (1992).

[11] A.L. Owczarek and T. Prellberg, J. Stat. Phys. **70**, 1195 (1993).
[12] G.S. Joyce and A.J. Guttmann, J. Phys. A **27**, 4359 (1994).
[13] D. Dhar, M.H. Phani, and M. Barma, J. Phys. A **15**, L279 (1982) .
[14] T.T. Wu, B.M. McCoy, C.A. Tracy, and E. Barouch, Phys. Rev. B **13**, 316 (1976).
[15] R.J. Baxter and A.J. Guttmann, J. Phys. A **21**, 3193 (1988).
[16] A.R. Conway, R. Brak, and A.J. Guttmann, J. Phys. A **26**, 3085 (1993).
[17] R.P. Stanley, Europ. J. Comb. **1**, 175 (1980).
[18] R.J. Baxter, in *Fundamental Problems in Statistical Mechanics,* edited by E.G.D. Cohen (North-Holland, Amsterdam, 1980), Vol. 5.
[19] D. Hansel, J.M. Maillard, J. Oitmaa, and M.J. Velgakis, J. Stat. Phys. **48**, 69 (1987).
[20] M.T. Jaekel and J.M. Maillard, J. Phys. A **18**, 1229 (1985).
[21] I.G. Enting, Ph.D. thesis, Monash University, 1973.
[22] A.J. Guttmann and I.G. Enting, Nucl. Phys. (Proc. Suppl.) (to be published).
[23] I.G. Enting, Nucl. Phys. (Proc. Suppl.) (to be published).
[24] G.E. Andrews, *q-Series: Their Development and Application in Analysis, Number Theory, Combinatorics, Physics, and Computer Algebra,* CBMS Regional Conference Lecture Ser. 66 (Am. Math. Soc., Providence, RI, 1986).
[25] G.E. Andrews, R.J. Baxter, and P.F. Forrester, J. Stat. Phys. **35**, 193 (1984).
[26] A.R. Conway (private communication).
[27] A.J. Guttmann and I. Jensen (to be published).